Perfluorotributylamine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.36

Global applicability domain: Outside

Local applicability domain index: 1.60e-01

Confidence level: 4.71e-01

Nearest Neighbors from the Training Set

Image not found
1-Hexadecyl-2,4-dimethylpyridin-1-ium iodide
Measured: 3.90
Predicted: 4.51

Image not found
1-Hexadecyl-3,4-dimethylpyridin-1-ium iodide
Measured: 3.16
Predicted: 3.41

Image not found
1-Hexadecyl-3,5-dimethylpyridin-1-ium iodide
Measured: 3.35
Predicted: 3.41

Image not found
1-Octadecylpyridin-1-ium iodide
Measured: 3.68
Predicted: 4.50